Microstructural Analysis of Thin Films Using X-ray Diffraction Techniques

Synchrotron X-ray diffraction measurements performed on the high-resolution powder diffraction beamline (BM16) at the European Synchrotron Radiation Facility (ESRF) have been used to study the microstructural properties of [111] oriented gold thin films. X-ray diffraction line profile measurements from the gold thin films revealed line broadening due to particle size effects, dislocations and stacking faults. From accurate lattice parameter measurements, application of a suitable macrostrain model showed planes inclined with respect to the substrate were in a state of compression. Furthermore, stacking faults populating inclined (111) planes were attributed to the residual scatter in the measured lattice parameters. Contrary to Transmission Electron Microscopy (TEM) results, the symmetry of the recorded profiles suggested negligible twin fault concentrations. Following a first-principles approach, based on the equivalent dislocation models of Wilkins and Krivoglaz, the dislocation character (i.e. edge, screw) and dislocation density in the gold films were evaluated. For all the films an optimized model consisted of mixed dislocations populating inclined (111) planes with a high dislocation density ranging from 10^{15} to 10^{16} m^{-2}. These results were found to be in approximate agreement with TEM analysis. This work also identified several shortcomings of the Wilkins dislocation model, such as the strong correlation between the dislocation density and the effective dislocation cut-off radius, and the inability to assign physical meaning to the model parameters. Finally, an overview of this work will be treated in view of recent literature in the field of dislocation analysis of thin films based on micro x-ray diffraction techniques.